Magnetic behavior of a non-extensive S-spin system: possible connections to manganites

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We analyzed the magnetic behavior of a S-spin system within framework of the Tsallis nonextensive statistics, employing the normalized approach. Unusual properties on magnetization, entropy and susceptibility emerge, as a consequence of nonextensivity. We further show that the nonextensive approach can be relevant to the field of manganites, materials which exhibit long-range interactions and fractality, two basic ingredients for nonextensivity. Our results are in qualitative agreement to experimental data in $La_{0.67}Ca_{0.33}MnO_3$ and $Pr_{0.5}Ca_{0.5}Mn_{0.95}Ga_{0.05}O_3$ manganites.

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I. INTRODUCTION

In 1988, Tsallis[1] proposed a q-dependent entropy functional which generalized the standard Maxwell-Boltzmann definition, to include non-extensive systems. In this formalism, "q" is called the *entropic index*, and measures the degree of nonextensivity of the system. A few years latter, Curado and Tsallis[2] revised the formalism introducing the *unormalized* constraint to the internal energy and showed that from this entropy functional a nonextensive thermodynamics could be derived. This generalization included the classical thermodynamics (Maxwell-Boltzmann), which could be recovered when q is set to unity.

After Curado and Tsallis work, this formalism has been successfully applied to various physical systems, where Maxwell-Boltzmann framework fails. These include: self-gravitating systems[3, 4], turbulence[5, 6, 7, 8], anomalous diffusion[9, 10, 11, 12], velocities of galaxies[13], solar neutrinos[14], etc.

In spite of these successes, some drawbacks were identified in the early formalism, namely: (a) the density operator was not invariant under a uniform translation of energy spectrum; (b) the q-expected value of the identity operator was not the unity; (c) energy was not conserved[15]. In a more recent work, Tsallis et al.[15] circumvent these difficulties introducing the *normalized* constraint to the internal energy of the system.

Concerning applications to magnetic systems, the unormalized formalism was used by Portesi et al.[16] and Nobre et al.[17], to describe the paramagnetic behavior of a system with N spins 1/2. The authors found a non-measurable magnetic susceptibility, since it was exponentially dependent on the number N of particles. Martínez et al.[18] analyzed the same S=1/2 system in the framework of the normalized formalism[15], finding a similar result to that reported by the Portesi et al. and Nobre et al.

In the present work, we analyzed the paramagnetic behavior of N spins S, within the normalized formalism and showed that the system effective temperature T does not relate with the inverse of the Lagrange multiplier β, as it is normally assumed, but with the inverse of a rescaled parameter β^* ($T = 1/k\beta^*$), already introduced by Tsallis[15]. In this approach, the unreal result found by Portesi[16], Nobre[17] and Martínez[18] was no longer found and the susceptibility became proportional to number of particles, as it is experimentally expected. In these early works, no attempt was made to correlate theoretical results to experimental magnetic systems of any kind.

We also suggest that the manganites are physical systems where the present concepts can be tested. Experimental data of Amaral et al.[19] and Hébert et al.[20], are in qualitative agreement with the results here reported. An analysis of non-extensivity in manganites in the ferromagnetic phase, also taking $T = 1/k\beta^*$ as an effective temperature, was already published elsewhere[21].

II. THE MODEL

We consider the Hamiltonian of a single spin S in a static and homogeneous magnetic field:

$$\hat{\mathcal{H}} = -\hat{\vec{\mu}} \cdot \vec{B} = -\hat{\mu}_z B = -g\mu_{\rm B} \hat{S}_z B \qquad (1)$$

where g=2, for J=S. The q-generalized magnetic moment thermal average $\langle \hat{\mu}_z \rangle_q$ is:

$$\langle \hat{\mu}_z \rangle_q = g\mu_{\rm B} \langle \hat{S}_z \rangle_q = g\mu_{\rm B} S B_{\rm S}^{(q)} \qquad (2)$$

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where $\langle\hat{S}_z\rangle_q$ is q-generalized thermal average spin operator and $B_S^{(q)}$ is the *generalized Brillouin function*. This first quantity can be determined in the Tsallis framework of normalized q-expectation values[15], from:

$$\langle\hat{S}_z\rangle_q = \frac{Tr\{\hat{\rho}^q\hat{S}_z\}}{Tr\{\hat{\rho}^q\}} \tag{3}$$

where $\hat{\rho}$ is the density operator, derived from the maximization of the entropy. Below, we analyze two different proposals for the entropy and show that re-scaling the Lagrange parameter, the same density operator emerges from both definitions.

A. Tsallis Entropy

The entropy of the system is defined as[1, 2, 15]:

$$\mathcal{S}_q = Tr\{\hat{\rho}^q\hat{\mathcal{S}}_q\} = \frac{k}{(q-1)}[1 - Tr\{\hat{\rho}^q\}] \tag{4}$$

where,

$$\hat{\mathcal{S}}_q = -k\ln_q\hat{\rho} \tag{5}$$

and k a positive constant. The generalized logarithm is defined as[22]:

$$\ln_q f = (1-q)^{-1}(f^{1-q} - 1) \tag{6}$$

The corresponding density operator $\hat{\rho}$ can be determined from the maximization of the $\mathcal{S}_q$ functional, subjected to q-normalized constraint[15]:

$$U_q = \frac{Tr\{\hat{\rho}^q\hat{\mathcal{H}}\}}{Tr\{\hat{\rho}^q\}} \tag{7}$$

and the normalization of density operator $Tr\{\hat{\rho}\} = 1$, leading to:

$$\hat{\rho} = \frac{1}{Z_q}\left[1 - (1-q)\frac{\beta}{Tr\{\hat{\rho}^q\}}(\hat{\mathcal{H}} - U_q)\right]^{\frac{1}{1-q}} \tag{8}$$

where Z_q is the generalized partition function:

$$Z_q = Tr\left\{\left[1 - (1-q)\frac{\beta}{Tr\{\hat{\rho}^q\}}(\hat{\mathcal{H}} - U_q)\right]^{\frac{1}{1-q}}\right\} \tag{9}$$

and β is the Lagrange parameter associated to internal energy constraint[15, 23]. In this case, the entropy has a well defined concavity, for any value of q, being concave for $q > 0$, and convex for $q < 0$[1, 2, 15, 23].

B. Normalized Tsallis Entropy

If the entropy functional $\hat{\mathcal{S}}_q$ is defined as proposed by Rajagopal and Abe[24]:

$$\mathcal{S}_q = \frac{Tr\{\hat{\rho}^q\hat{\mathcal{S}}_q\}}{Tr\{\hat{\rho}^q\}} = \frac{k}{(q-1)}\left[\frac{1}{Tr\{\hat{\rho}^q\}} - 1\right] \tag{10}$$

the density operator $\hat{\rho}$ can be determined in a similar way as above, yielding:

$$\hat{\rho} = \frac{1}{Z_q}\left[1 - (1-q)\beta Tr\{\hat{\rho}^q\}(\hat{\mathcal{H}} - U_q)\right]^{\frac{1}{1-q}} \tag{11}$$

$$Z_q = Tr\left\{\left[1 - (1-q)\beta Tr\{\hat{\rho}^q\}(\hat{\mathcal{H}} - U_q)\right]^{\frac{1}{1-q}}\right\} \tag{12}$$

In this case, the q parameter is restricted to the interval $0 \leq q \leq 1$, preserving the entropy concavity[24].

The density operators emerging from both cenarios (Eq.8 and 11) can be re-written in the form:

$$\hat{\rho} = \frac{1}{Z'_q}\left[1 - (1-q)\beta^*\hat{\mathcal{H}}\right]^{\frac{1}{1-q}} \tag{13}$$

$$Z'_q = Tr\left\{\left[1 - (1-q)\beta^*\hat{\mathcal{H}}\right]^{\frac{1}{1-q}}\right\} \tag{14}$$

where,

$$\beta^* = \frac{\beta}{Tr\{\hat{\rho}^q\} + (1-q)U_q\beta} \tag{15}$$

for the case A, and:

$$\beta^* = \frac{\beta}{\frac{1}{Tr\{\hat{\rho}^q\}} + (1-q)U_q\beta} \tag{16}$$

for case B. Here, we suggested that the effective temperature is:

$$T = \frac{1}{k\beta^*} \tag{17}$$

and the density operator becomes independent of the initial entropy functional.

The magnetic behavior of a S-spin system will be analyzed as a function of the parameter $x^* = g\mu_B SB\beta^*$. In fact, in terms of x^*, the generalized Brillouin function, is given by:

$$B_S^{(q)} = \frac{1}{S}\langle\hat{S}_z\rangle_q = \frac{1}{S}\frac{\sum\limits_{m_s=-S}^{+S} m_s\left[1 + (1-q)x^*\frac{m_s}{S}\right]^{\frac{q}{1-q}}}{\sum\limits_{m_s=-S}^{+S}\left[1 + (1-q)x^*\frac{m_s}{S}\right]^{\frac{q}{1-q}}} \tag{18}$$

It is to be remarked that cut-off procedure[23, 25, 26, 27] implies that those states that do not satisfy the condition:

$$1 + (1-q)x^* \frac{m_s}{S} \geq 0 \tag{19}$$

must be excluded from the summation. In other words, these states are assigned with a zero probability amplitude, preserving the positive definition of the density operator[16].

For a system constituted by N spins S particles the q-generalized spin operator thermal average (Eq.3), can be written as:

$$\langle \hat{S}_z \rangle_{q,N} = \frac{\sum\limits_{m_s=-NS}^{+NS} Y(m_s) m_s \left[1 + (1-q)x^* \frac{m_s}{S}\right]^{\frac{q}{1-q}}}{\sum\limits_{m_s=-NS}^{+NS} Y(m_s) \left[1 + (1-q)x^* \frac{m_s}{S}\right]^{\frac{q}{1-q}}} \tag{20}$$

where, $Y(m_s)$ is the multiplicity and :

$$\sum_{m_s=-NS}^{NS} Y(m_s) = (2S+1)^N \tag{21}$$

In the particular case of N 1/2-spins particles, $Y(m_s)$ is simply given by:

$$Y(m_s) = \frac{N!}{\left(\frac{N}{2} - m_s\right)! \left(\frac{N}{2} + m_s\right)!} \tag{22}$$

III. RESULTS AND DISCUSSION

When q is different from unity, general expressions for magnetic observables are difficult to calculate and interpret, even for simple systems. This hinders the comparison between theoretical predictions and experimental results. Numerical methods, on the other hand, provide a means to directly calculate observables, allowing a deeper understating of the theoretical results.

Figure 1 displays the generalized Brillouin function $B_{\mathrm{S}}^{(\mathrm{q})}$ vs. x^* (Eq.18), for different values of q and S=5/2. For q up to 0.5, a series of kinks appear in the curve. One also notes that the saturation value $B_{\mathrm{S}}^{(\mathrm{q})}|_{\mathrm{SAT}}$ decreases with decreasing q. This is more clearly shown in figure 2(a) and (b), where $B_{\mathrm{S}}^{(\mathrm{q})}|_{\mathrm{SAT}}$ is plotted as a function of q, for half-integer and integer spin values, respectively. The behavior of a classical spin is also included and can be exactly calculated from Eq.18 with $S \to \infty$, giving:

$$B_{\mathrm{S}}^{(\mathrm{q})}|_{\mathrm{SAT}} = \frac{1}{2-q} \tag{23}$$

The occupation probability (OP), as a function of x^*, for each energy level of S=5/2 are displayed in figure 3(a)(b)(c), for several values of q. Figure 3(d) shown the same quantity for S=2 and q=0.1. We observe that the OP does not vanish for negative energy levels ($m_s > 0$), even for very large values of x^*, in contrast to what happens in the case q=1 (Maxwell-Boltzmann). From figure 3(c) we can see that, for q=0.1, the OP of the positive energy states ($m_s < 0$) vanish sharply at the same x^* values as the kinks observed in figure 1. This occurs for q<0.5. Therefore, we correlate the kinks observed on the magnetization curves to the lost of occupation of the most energetic states. This is consequence of Tsallis' cut-off. In fact, from Eq.19, the x^* values where the kinks occurs can be derived, following:

$$x_{m_s}^{kinks} = \frac{S}{|m_s|(1-q)} \tag{24}$$

It is to be remarked that for a half-integer spin, S+1/2 kinks occur, and S for an integer spin.

Figure 4(a)(b) display, respectively, the unormalized (Eq.4) and normalized (Eq.10) entropy $\mathcal{S}_q$, for S=5/2 and different q values. Note that, for q<0.5, the kinks discussed before are present. Besides, for any q<1, the entropy does not vanish in the limit ${x^*}^{-1} \to 0$. In other words, even for high field and/or low temperature, the system has a finite entropy, which prevents a fully magnetized state. These features are valid for both entropy functionals (section II).

A general expression for the magnetic susceptiblity can be deduced from Eq.3 and Eq.18:

$$\chi_q = \lim_{B \to 0} \left[\frac{\partial \langle \hat{\mu}_z \rangle_q}{\partial B}\right] = \frac{C^{(q)}}{T} \tag{25}$$

where $C^{(q)} = qC^{(1)}$ is the generalized Curie constant. Figure 5 displays χ_q^{-1} as a function of ${x^*}^{-1}$ for q=1.0 and 0.8, with S=5/2.

In order to compare the predictions of the proposed model to experimental data, we must investigate how the magnetic observables discussed before scales upon increasing the number of particles in the system. An extensive quantity $\mathcal{F}$ scales as

$$\mathcal{F}_N = N \mathcal{F}_1 \tag{26}$$

where N is the system number of particle.

Particularly useful for the purpose of comparison, is the magnetic susceptibility. Portesi et al.[16] and Nobre et al.[17], considered the generalized magnetization on paramagnetic fase of a N 1/2-spin system in the unormalized formalism[2, 15, 16, 17, 23]. They found for χ_q:

$$\chi_q = \frac{C_{\mathrm{S}=1/2}^{(\mathrm{q})}}{T} 2^{N(1-q)} \tag{27}$$

where,

$$C^{(q)}_{S=1/2} = \frac{(g\mu_B)^2}{4k} Nq \tag{28}$$

and $T = 1/k\beta$ is the temperature of the system. Here, β is the usual Lagrange parameter associated to the non-normalized constraint of internal energy.

Therefore, as N increases, the magnetic susceptibility becomes infinity for q<1 and zero for q>1. In other words, there is no linearity among χ_q and N. This phenomenon is called *dark magnetism*, in analogy to the cosmological concept of *dark matter* [[16] and references there in].

S. Martínez et al.[18], analyzed the paramagnetic behavior of the same N 1/2-spin system, however, within the normalized formalism[15, 23], and found a similar result as Portesi and Nobre for χ_q.

Our proposal is that the paramagnetic behavior of a non-extensive N 1/2-spin system should be analyzed in the normalized formalism, using the density operator described in Eq.13, taking β^*, instead β, inversely proportional to the system temperature T. By doing so, the generalized paramagnetic susceptibility becomes:

$$\chi_q = \frac{C^{(q)}_{S=1/2}}{T} \tag{29}$$

which does not diverge as N increases, and is indeed proportional to N. Besides, this result is independent of the choice for the functional entropy.

IV. POSSIBLE CONNECTION TO EXPERIMENTAL RESULTS

Amaral et al.[19] discussed the magnetic behavior of manganese oxides, namely, $La_{0.67}Ca_{0.33}MnO_3$ and verified steps on the curve of M^{-1} vs. T in the paramagnetic phase, as shown in figure 6(a). These steps are analogue to those shown on figure 6(b), that represents also the inverse of magnetization as a function of x^{*-1}, for q=0.1, and encourage the idea of manganites as non-extensive objects[21]. The authors relate the change in the slope of the curve as an indication of cluster formation, which change the effective moment of Mn ions. These clusters could give rise to fractal structures, as discussed by Dagotto[28], and therefore are in accordance to the ideas discussed here.

In addition, Hébert et al.[20] found magnetization curves in $Pr_{0.5}Ca_{0.5}Mn_{0.95}Ga_{0.05}O_3$ that are also in qualitative agreement to those curves in figure 1.

V. CONCLUSION

In summary, we investigated the properties of a paramagnetic S-spin system under Tsallis generalized statistics, on the normalized formalism. For q<0.5, a series of kinks appears in magnetization and entropy. This effect is a direct consequence of a peculiar occupation probability, as a result of Tsallis' cut-off, where the positive energy states ($m_s < 0$) vanish sharply. Additionally, the negative energy states ($m_s > 0$) share non-zero occupation probability, preventing a fully magnetized state and the saturation magnetization decreases with decreasing q. We present evidences based on experimental results of Amaral et al.[19] and Hébert et al.[20] which add and support our previous publication[21], where manganites are suggested to be magnetically non-extensive objects.

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VI. CAPTIONS

Figure 1: Generalized Brillouin function for several q values and S=5/2, as a function of x^*.

Figure 2: Saturation magnetization $B^{(q)}_S|_{SAT}$ as a q function, for (a)half-integer and (b)integer S values.

Figure 3: Probability of occupation of each energy level, for (a)(b)(c) S=5/2 and (d) S=2, as a function of x^*, and various values of q.

Figure4: (a) Unormalized (Eq. 4) and (b) normalized (Eq. 10) entropy $\mathcal{S}_q$, for S=5/2 and different q values, as a function of $x^{*^{-1}}$.

Figure5: Inverse of susceptibility for (a) q=1.0 and 0.8, for S=5/2, as a $x^{*^{-1}}$ function.

Figure6: (a) Temperature dependence of the inverse susceptibility for the manganite La2/3Ca1/3MnO3, above the Curie temperature (267 K), at low magnetic field. (b)Inverse of magnetization (Eq.18) as a function of x^{*-1}, for q=0.1

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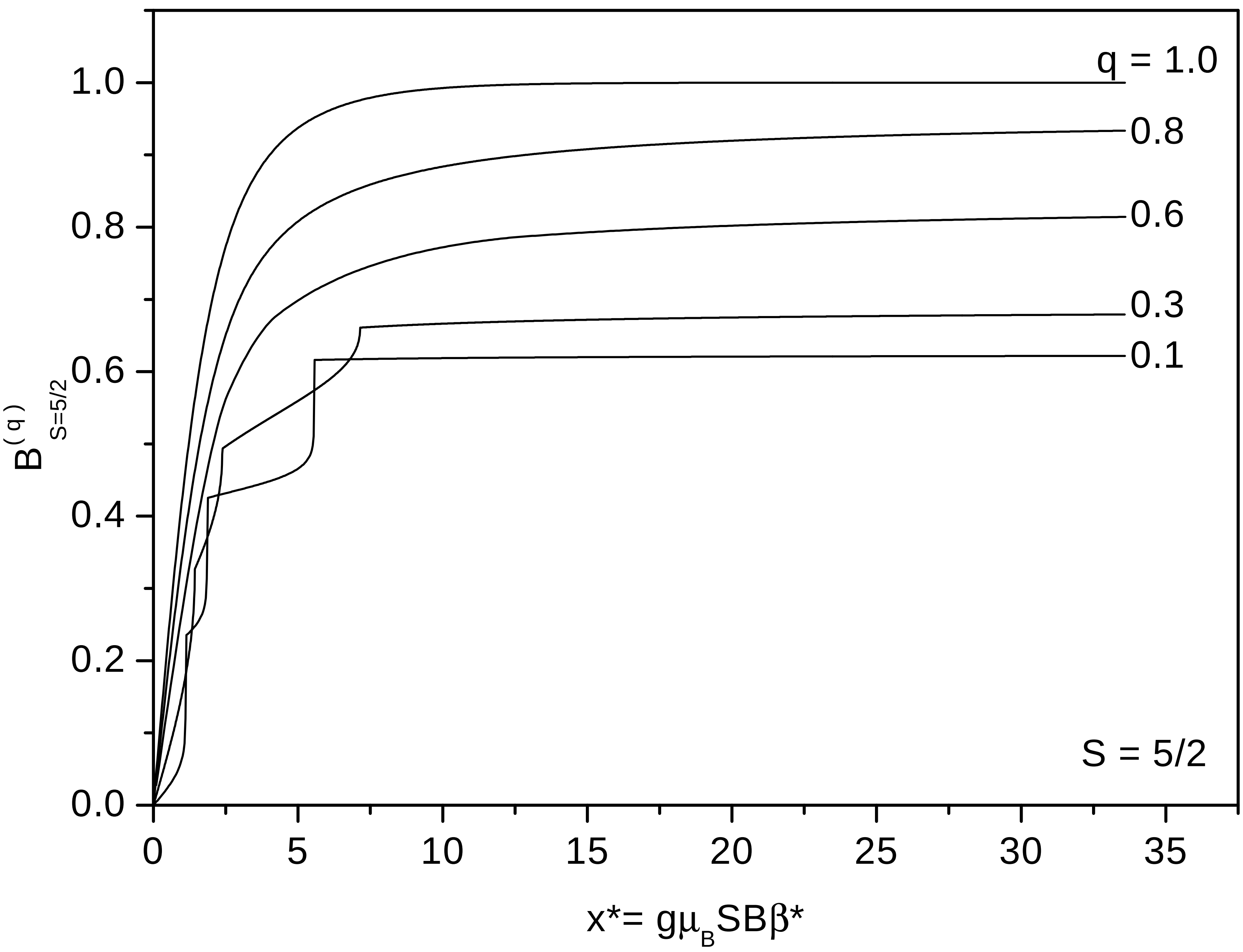


Figure 2 - M.S. Reis *et al.*

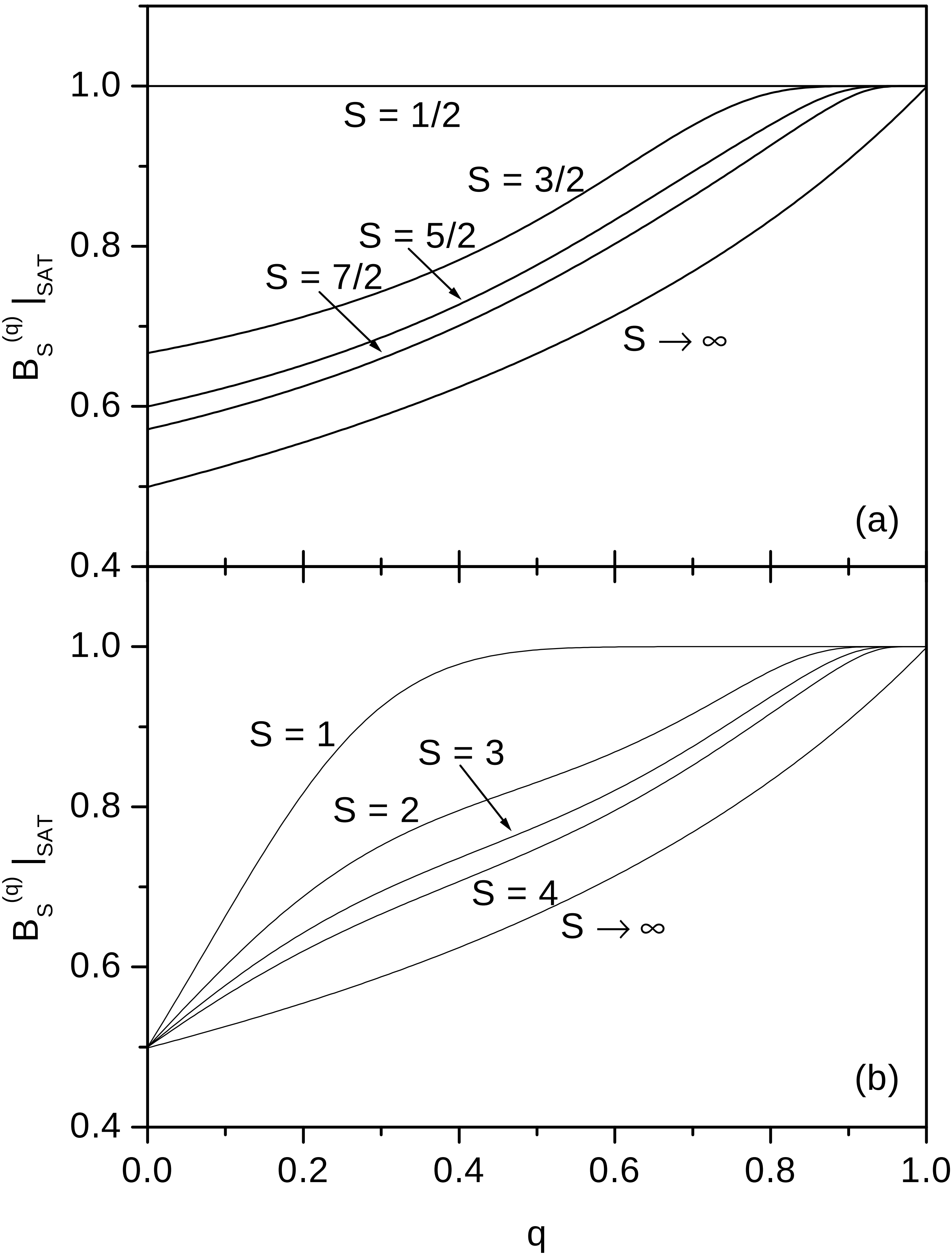


Figure 3 - M.S. Reis *et al.*

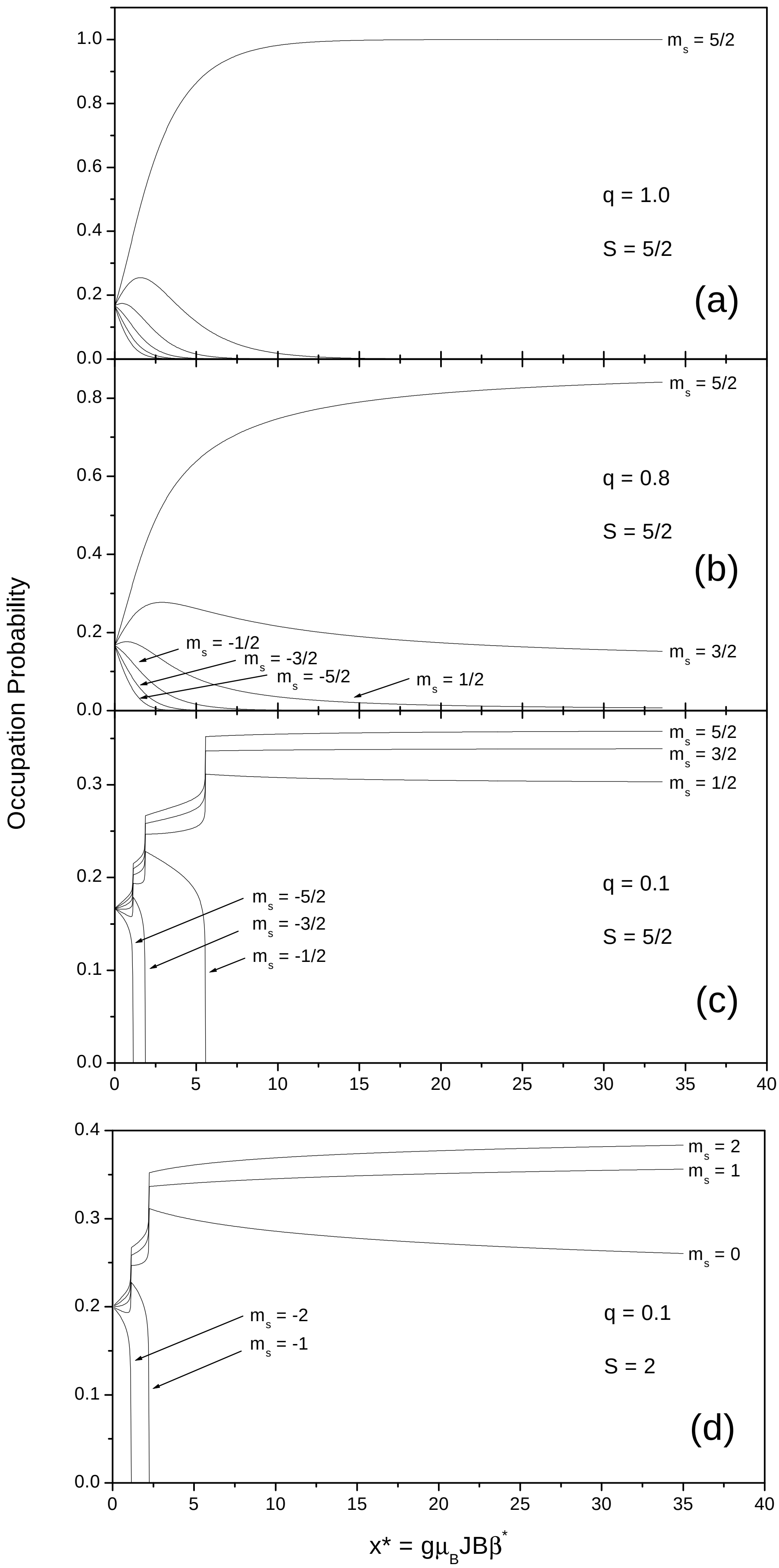
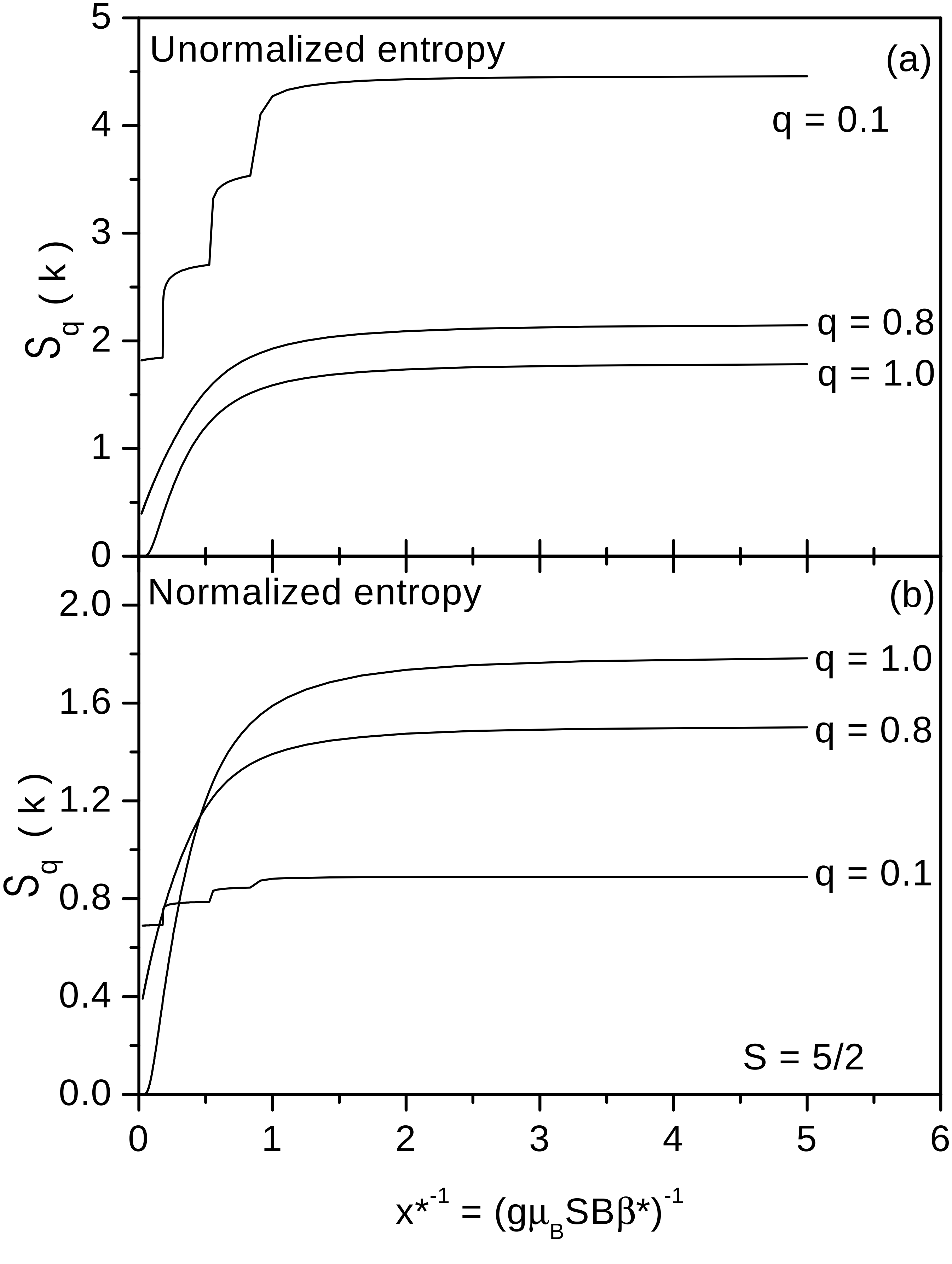


Figure 4 - M.S. Reis *et al.*



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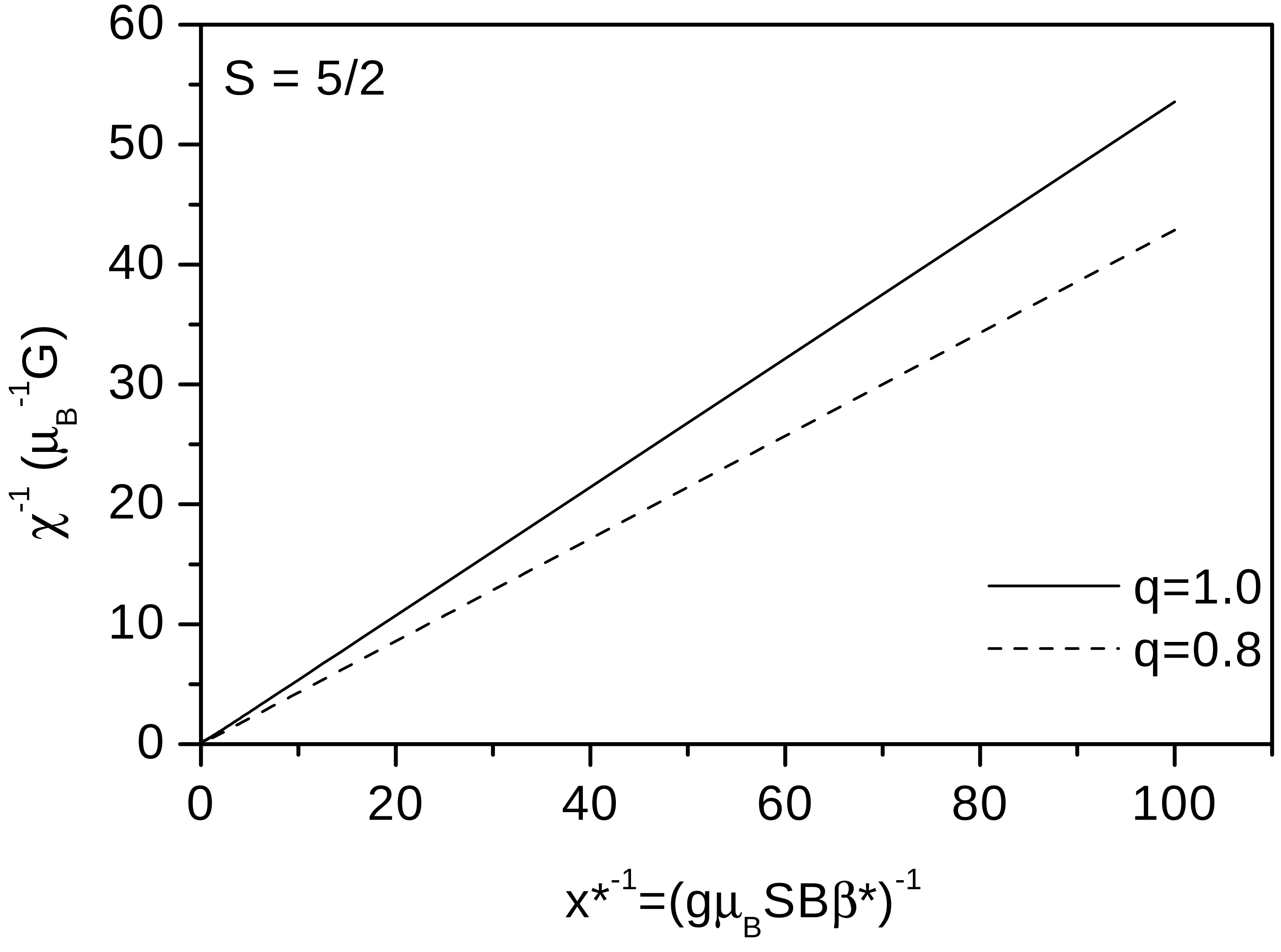

Figure 6 - M.S. Reis *et al.*